TITLE: Numerical Efficiency of Explicit and Implicit Methods with Multigrid for Large Eddy Simulation

NUMERICAL EFFICIENCY OF EXPLICIT AND IMPLICIT METHODS WITH MULTIGRID FOR LARGE EDDY SIMULATION

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Abstract. In this paper the accuracy and efficiency of a finite-volume multigrid solver for Large Eddy Simulation (LES) is investigated. The spatial discretization method employed is a second-order accurate central differencing scheme. For time discretization of the momentum equations the implicit second-order Crank-Nicolson method and the explicit second-order Adams-Bashforth method are considered. The influences of the two time discretizations, choice of grid size and time-step size and multigrid performance on the numerical accuracy and computational efficiency are discussed.

1. Introduction

Due to the foreseeable progresses in the performance of computer systems, it can be expected, that in the near future the Large Eddy Simulation (LES) will become more important and applicable also in industrial practice. However, efficient numerical algorithms designed for modern parallel computer architectures with facilities to allow the modeling of complex geometries are another crucial issue in the application of LES. In this way it will be possible to achieve a sufficient numerical resolution and geometrical flexibility also to deal with complex practical problems within reasonable computing times.

Numerical aspects such as spatial and temporal discretization, solution algorithms and resolution requirements , and modeling aspects such as subgrid scale models are effecting the accuracy and efficieny of the simulations. Due to the enormous computational requirements for LES, there can be found few systematic investigations about the above mentioned aspects. Despite that different groups have organized LES workshops for specified test cases, it was difficult to come to any definite conclusions about the performance of different applied numerical methods as well as the varying subgrid scale models.

In this study the accuracy and performance of a finite-volume multigrid solver for LES is investigated. The main focus of the present contribution will relate to the following aspects with respect to their influences on the numerical accuracy and computational efficiency of the considered approach: comparison of the explicit/implicit methods, choice of grid size and time-step size and multigrid performance.

For this an already well investigated turbulent channel flow will be considered for comparison to other results from the literature.

2. Numerical Procedure

The governing equations for an incompressible flow are given by

$$\frac{\partial \bar{u}_i}{\partial x_i} = 0, \tag{1}$$

$$\frac{\partial(\rho\bar{u}_i)}{\partial t} + \frac{\partial\left(\rho\bar{u}_i\bar{u}_j\right)}{\partial x_j} = -\frac{\partial\bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j}\left[\mu\left(\frac{\partial\bar{u}_i}{\partial x_j} + \frac{\partial\bar{u}_j}{\partial x_i}\right)\right] - \frac{\partial\tau_{ij}}{\partial x_j}, \tag{2}$$

where $\bar{u}_i$ are the velocity components of the resolved scales with respect to the Cartesian coordinates x_i, $\bar{p}$ is the corresponding pressure, μ is the viscosity, ρ is the density and t is the time. The subgrid scale stresses

$$\tau_{ij} = \rho\left(\overline{u_i u_j} - \overline{u}_i\overline{u}_j\right) \tag{3}$$

are modeled by the Smagorinsky model [1] and the dynamic Germano model [2] to close the problem. In order to stabilize the dynamic model, the negative values for the parameter C_s of the underlying Smagorinsky model are clipped.

The basic flow solver is the FASTEST-3D code (INVENT Computing, Erlangen) [3] with extensions for LES. The solver is based on a fully conservative finite-volume method for solving the incompressible Navier-Stokes equations on a non-staggered, cell-centered grid arrangement. The spatial discretization method employed is a second-order accurate central differencing scheme for block-structured non-orthogonal boundary-fitted grids. For time discretization of the momentum equations we consider two different approaches: the implicit second-order Crank-Nicolson method and the explicit second-order Adams-Bashforth method. Both methods define approximations $\bar{u}_h^n$ and $\bar{p}_h^n$ to the solution of the continuous problem at the time levels $t_n = n\Delta t \quad (n = 1, 2, ...)$, where the parameter h is a measure for the spatial resolution and $\Delta t > 0$ is the time-step size.

Within the implicit method, for each time-step, assuming that the unknowns at the time level t_{n-1} have already been computed, the unknowns at the time level t_n have to be determined as the solution of a nonlinear algebraic system. For this a nonlinear full approximation multigrid scheme with a pressure-correction smoother is employed [4].

The smoothing procedure is based on a variant of the well-known SIMPLE algorithm proposed by Patankar and Spalding [5]. The determination of $\bar{u}_h^n$ and $\bar{p}_h^n$ is done in several steps. In the first step, after the calculation of the turbulent viscosity, an intermediate approximation to $\bar{u}_h^n$ is obtained by solving the discrete momentum equations with the pressure term, the source term and the matrix coefficients formed with values of the previous iteration. In the second step, corrections $\Delta\bar{p}_h^n$ and $\Delta\bar{u}_h^n$ are sought to obtain the new pressure $\bar{p}_h^n$ and the new velocity $\bar{u}_h^n$ exactly satisfying the continuity equation. By considering a modified discrete momentum equation together with the discrete continuity equation, an equation for the pressure correction $\Delta\bar{p}_h^n$ is derived, where a selective interpolation technique is used for making the cell face velocities dependent on the nodal pressure, which is necessary to avoid oscillatory solutions that may occur owing to the non-staggered grid arrangment[6]. To improve the diagonal dominance in the pressure-correction equation the contributions due to grid non-orthogonality are neglected. The smoothing iteration step is completed by correcting the velocity components and the pressure. To ensure convergence, for the velocity components and the pressure an under-relaxation in the variant suggested by Patankar [7] is employed. For the solution of the linear system of equations the Strongly Implicit Procedure (SIP) of Stone [8] is used. The global outer multigrid procedure is implemented as a nonlinear full approximation scheme, in which the above pressure-correction scheme acts as the smoother. The different grid levels are visited following the standard V-cycle approach, where second-order interpolation is employed for the grid transfers. This procedure is repeated till convergence is reached.

Within the explicit method, first the turbulent viscosity and the velocity $\bar{u}_h^n$ are calculated explicitly from the unknowns at the time level t_{n-1}. Then the pressure correction equation is derived using the modified discrete momentum equation together with the discrete continuity equation. The corresponding resulting linear system is solved by a linear multigrid method. The computation of the time level t_n is completed by correcting the velocity components and the pressure. In Figure 1 a schematical flow diagram of both methods is given.

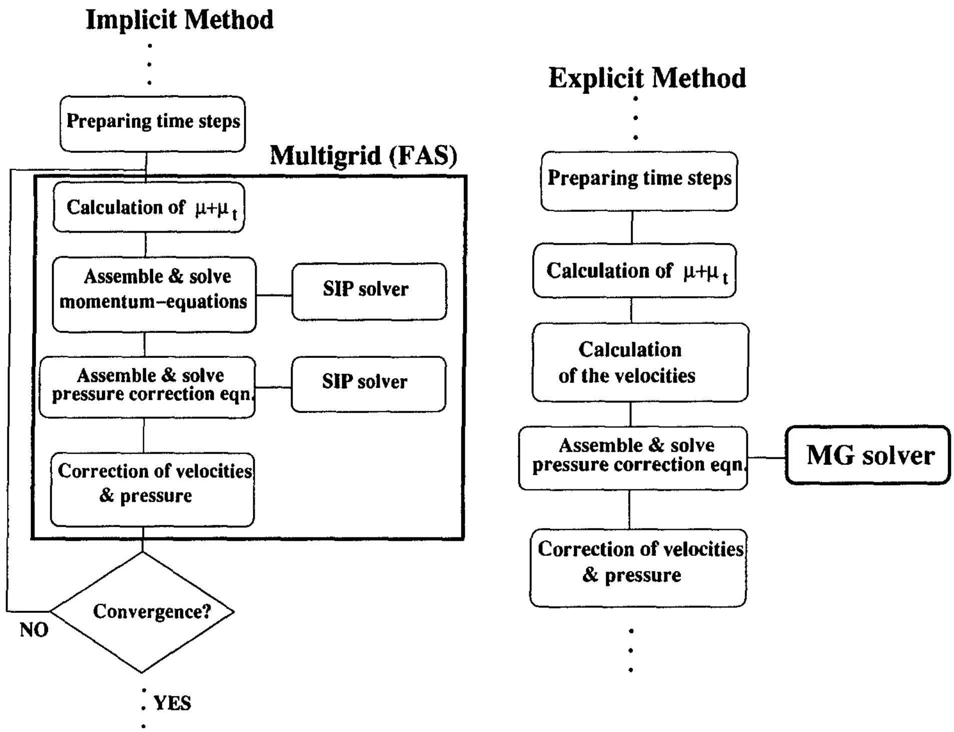

Figure 1. Flow diagram of implicit/explicit methods.

3. Numerical Results

The following investigations concern the accuracy and the numerical efficieny of the methods given in the previous section. All computations were carried out on a Compaq AlphaServer ES40 667 MHz.

As a test case the turbulent flow between two parallel plates seperated by a distance 2δ is investigated. The flow is driven by a uniform streamwise pressure gradient. The Reynolds number $Re_\tau = 395$ $(Re_b = 6875)$ based on half-width and friction (or bulk) velocity is considered. Since the streamwise and spanwise directions (i.e. x and z) are formally infinite, periodic boundary conditions are used for the simulation of a finite domain. The computational domain has the dimensions $2\pi\delta \times 2\delta \times \pi\delta$ which are considered to be large enough to avoid adverse effects of the periodic boundary conditions. Initial conditions with random fluctuations are given to assure turbulence. Three different grids with $64 \times 32 \times 32$, $96 \times 48 \times 48$ and $128 \times 64 \times 64$ control volumes (CVs) are employed in x, y, z directions. The grids are equidistant in streamwise and spanwise directions where in the wall-normal direction a geometric progression is used for the grid density. The first point away from the wall is at $y^+ \approx 9.25$ for the coarse grid,

$y^+ \approx 6.17$ for the medium grid and $y^+ \approx 4.62$ for the fine grid. Before starting the computation of mean values and statistics of the flow, the simulations are carried out until the numerical solution reached a statistically steady state. All data are computed from the appropriate quantities and averaged in the homogeneous spatial directions x and z and in time. The averages in time are taken over 200 s in each case. The results are compared to the DNS data given in [9].

First, a validation of the applied subgrid models is carried out. In Figure 2 (left) a comparison of the mean velocity profile U_m normalized by the friction velocity u_τ in the normalized half channel width is given. The results

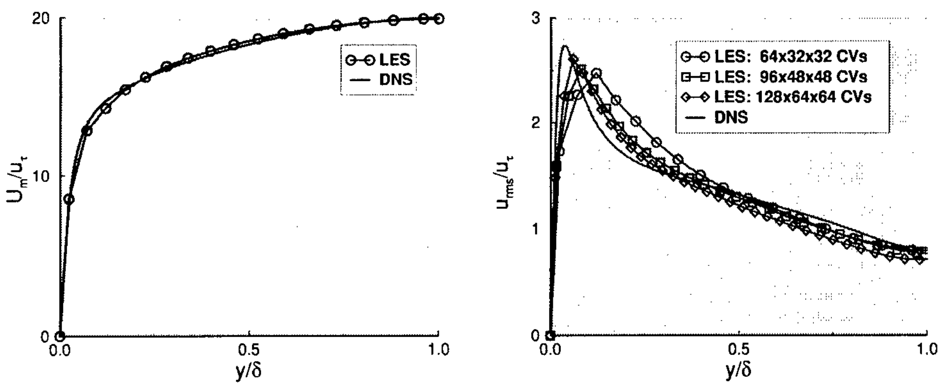

Figure 2. Comparison of mean velocity profile (left) and rms velocity profile (right) between LES and DNS.

calculated with the finest grid and the Germano model correspond well with the reference data. Figure 2 (right) shows the root mean square u_{rms} of the velocity in streamwise direction normalized by the friction velocity u_τ in normalized half channel width for three grids with the Smagorinsky model. Compared with the DNS data the LES results for the coarse grid show slightly lower fluctuations. However, the overall agreement is satisfactory and with grid refinement the profile approaches the reference data.

Next, the numerical efficiencies of the explicit and implicit methods are investigated. Figure 3 shows the comparison of both methods without the multigrid solver for CFL=0.5, where the computational time per time-step against the number of CVs is plotted. The CFL-number is defined by

$$\mathrm{CFL} = \max_{\mathrm{CV}} \left[\sum_{i=1}^{3} \bar{u}_i / \Delta x_i \right] \cdot \Delta t \,,$$

where the maximum is taken over all control volumes (CV). It is observed that without a multigrid solver the implicit method is more efficient than

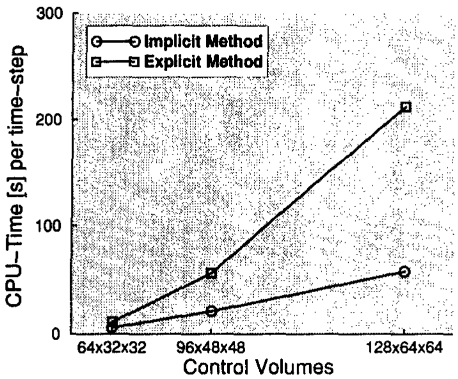

Figure 3. Comparison of explicit and implicit methods without the multigrid solver for CFL=0.5 with varying grid size.

the explicit method, where the differences in CPU-time increase with grid refinement. This is due to the fact, that within the explicit method, the pressure-correction equation has to be solved very exactly, since it is solved only once. Thus the CPU-time for solving the linear system without the multigrid solver is very high and the computational effort increases rapidly when the grid is refined.

In Figure 4 the computational time per time-step against the number of CVs for both methods with the multigrid solver for the same CFL-number is plotted. The multigrid approach yields an acceleration for both methods. The acceleration for the explicit method is much higher as for the implicit method, such that the explicit method becomes superior to the implicit one.

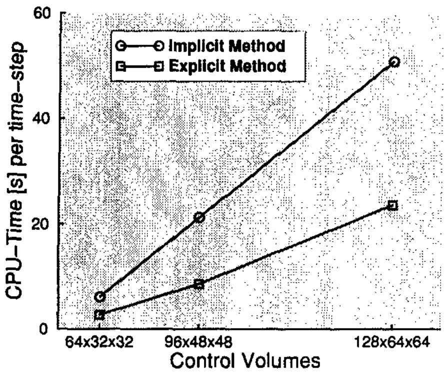

Figure 4. Comparison of explicit and implicit methods with the multigrid solver for CFL=0.5 with varying grid size.

Since there exists no strict time-step limitation, of course, with the implicit method computations with higher CFL numbers are possible. In Figure 5 the computing times against the number of CVs are plotted for the implicit method using CFL=6 and the explicit method using CFL=0.5. It can be seen that even in this comparison the explicit method still turns out to be slightly more efficient. In order to see how the time-step size is effecting the results of the computations, in Figure 6 the root mean square values u_{rms} of the velocity in streamwise direction normalized by the friction velocity u_τ in the normalized half channel width for the coarse grid with the Smagorinsky model is shown for different CFL-numbers. The computations with a larger time-step size (CFL=6) overpredict the streamwise fluctuations when compared with the smaller time-step size (CFL=0.5). Further test computations have shown that using even larger time-step sizes (e.g. CFL=10) yield rather poor results, such that for the considered test case CFL=6 can be viewed as the maximum value to achieve physically reasonable results.

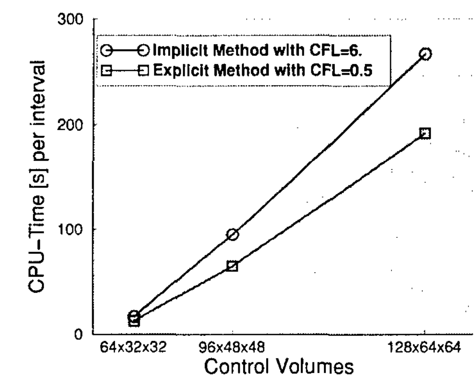

Figure 5. Comparison of explicit and implicit methods with the multigrid solver for different CFL-numbers and varying grid size.

4. Conclusions

The numerical accuracy and efficieny of explicit and implicit methods with and without multigrid for Large Eddy Simulation has been investigated. For the comparisons the simple well known turbulent channel flow is considered. Without using the multigrid solver, the computational requirement for the explicit method increases very rapidly with increasing number of grid points, such that in this case the implicit method is superior. However, when employing the multigrid solver, a high acceleration for the explicit method can be realized, which makes the method more efficient than the implicit one. It has been shown, that with the implicit method it is possible

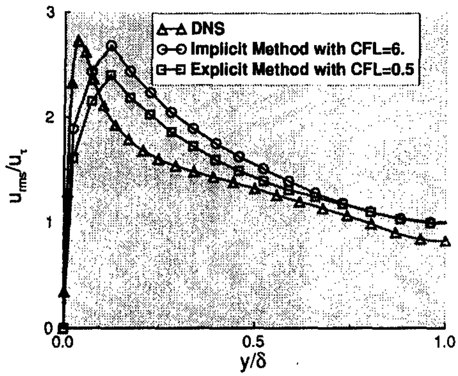

Figure 6. Comparison of rms velocity profile for different CFL-numbers.

to achieve also for CFL>1 physically reasonable results, but comparing the overal computational performance the explicit method still turned out to be superior.

Of course, it would be of interest, if the findings for the considered geometrically very simple test case will also be confirmed for problems in more complex geometries. The situation may change in such cases, when it is necessary to use more irregular grids with higher variations of control-volume sizes. Here, the advantages of the implicit method, where there is no need to adjust the time-step size to the smallest control volumes, can become more dominant. Corresponding investigations will be a topic of forthcoming work.

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